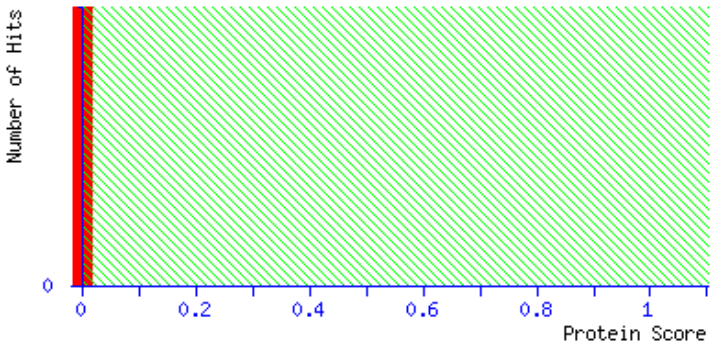
Mascot Search Results

```
User            : Lily-mascot
Email           : l.r.adair@pgr.reading.ac.uk
Search title    : Peptide mix chimeric MS/MS m/z 1047 (03072023)
MS data file    : 1047.txt
Database        : SwissProt 2021_01 (564277 sequences; 203340877 residues)
Taxonomy        : Eukaryota (eucaryotes) (192754 sequences)
Timestamp       : 3 Jul 2023 at 13:35:13 GMT
```

Mascot Score Histogram

Ions score is -10*Log(P), where P is the probability that the observed match is a random event.
Individual ions scores > 51 indicate identity or extensive homology (p<0.05).
Protein scores are derived from ions scores as a non-probabilistic basis for ranking protein hits.



Peptide Summary Report

Format As Peptide Summary Help

Significance threshold p< 0.05 Max. number of hits AUTO

Standard scoring MudPIT scoring Display non-significant matches Show sub-sets 0

Show pop-ups Suppress pop-ups Sort unassigned Decreasing Score Require bold red

Preferred taxonomy All entries

Select All Select None Search Selected Error tolerant Archive Report

No significant hits to report

Peptide matches not assigned to protein hits: (no details means no match)

	Query	Observed	Mr(expt)	Mr(calc)	ppm	Miss	Score	Expect	Rank	Unique	Peptide
☑	2	2093.0862	2092.0789	2092.0789	0.03	0	38	1	1		SYSMEHFRWGKPVGKKR
☑	1	1046.5418	1045.5345	1045.5444	-9.46	0	21	54	1		FSPLDSPKGV

Search Parameters

```
Type of search         : MS/MS Ion Search
Enzyme                 : None
Mass values            : Monoisotopic
Protein Mass           : Unrestricted
Peptide Mass Tolerance : ± 10 ppm
Fragment Mass Tolerance: ± 0.2 Da
Max Missed Cleavages   : 0
Instrument type        : MALDI-QUAD-TOF
Number of queries      : 2
```

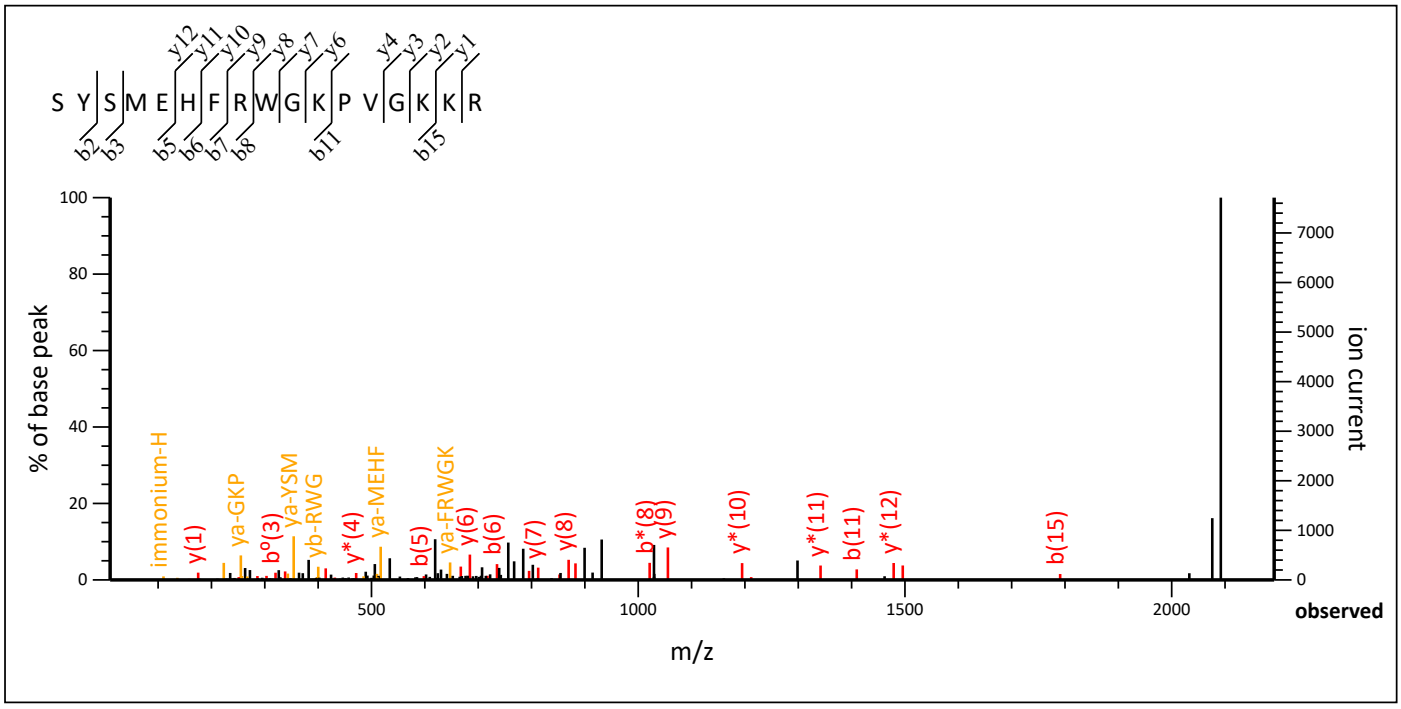
Mascot: http://www.matrixscience.com/

Mascot Search Results

Peptide View

MS/MS Fragmentation of **SYSMEHFRWGKPVGKKR**
Found in **COLI_BALBO** in **SwissProt**, Pro-opiomelanocortin (Fragment) OS=Balaenoptera borealis OX=9768 GN=POMC PE=1 SV=1

Match to Query 2: 2092.078924 from(2093.086200,1+) intensity(1.0000) index(0)
Title: Reading Top-Down experiment
Data file 1047.txt



10.07 to 2192.1

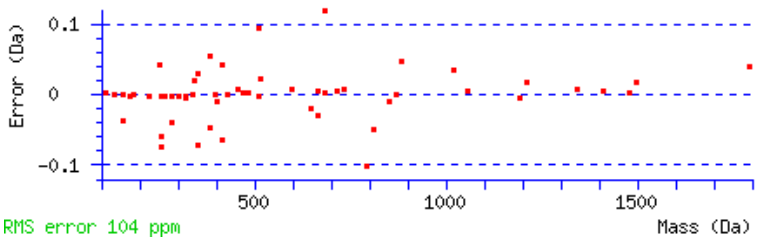
Label all possible matches ○ Label matches used for scoring ◉

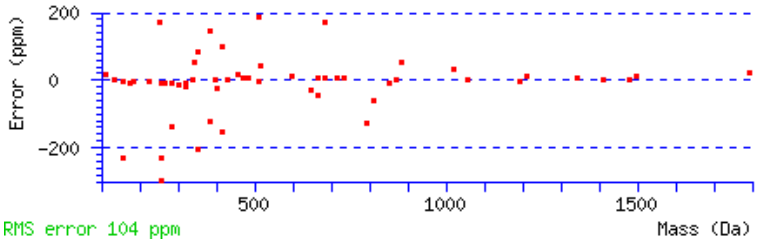
Monoisotopic mass of neutral peptide Mr(calc): 2092.0789
Ions Score: 38 **Expect:** 1
Matches : 65/200 fragment ions using 97 most intense peaks (help)

#	Immon.	b	b*	b^0	Seq.	y	y*	y^0	#
1	60.0444	88.0393		70.0287	S				17
2	136.0757	***251.1026***		233.0921	Y	2006.0541	1989.0276	1988.0436	16
3	60.0444	***338.1347***		320.1241	S	1842.9908	1825.9643	1824.9802	15
4	104.0528	469.1751		451.1646	M	1755.9588	1738.9322	1737.9482	14
5	102.0550	***598.2177***		580.2072	E	1624.9183	1607.8917	1606.9077	13
6	110.0713	***735.2767***		717.2661	H	***1495.8757***	1478.8491		12
7	120.0808	***882.3451***		864.3345	F	1358.8168	1341.7902		11
8	129.1135	1038.4462	1021.4196	1020.4356	R	***1211.7484***	1194.7218		10
9	159.0917	1224.5255	1207.4989	1206.5149	W	***1055.6473***	1038.6207		9
10	30.0338	1281.5470	1264.5204	1263.5364	G	***869.5679***	852.5414		8
11	101.1073	***1409.6419***	1392.6154	1391.6314	K	***812.5465***	795.5199		7
12	70.0651	1506.6947	1489.6681	1488.6841	P	***684.4515***	667.4250		6
13	72.0808	1605.7631	1588.7365	1587.7525	V	587.3988	570.3722		5
14	30.0338	1662.7846	1645.7580	1644.7740	G	488.3303	471.3038		4

15	101.1073	*1790.8795*	1773.8530	1772.8690	K	*431.3089*	414.2823		3
16	101.1073	1918.9745	1901.9479	1900.9639	K	*303.2139*	286.1874		2
17	129.1135				R	*175.1190*	158.0924		1

Seq	ya	yb	Seq	ya	yb	Seq	ya	yb
YS	223.1077	251.1026	YSM	354.1482	382.1431	YSME	483.1908	511.1857
YSMEH	620.2497	648.2446	SM	191.0849	219.0798	SME	320.1275	348.1224
SMEH	457.1864	485.1813	SMEHF	604.2548	632.2497	ME	233.0954	261.0904
MEH	370.1544	398.1493	MEHF	517.2228	545.2177	MEHFR	673.3239	
EH	239.1139	267.1088	EHF	386.1823	414.1772	EHFR	542.2834	570.2783
HF	257.1397	285.1346	HFR	413.2408	441.2357	HFRW	599.3201	627.3150
HFRWG	656.3416	684.3365	FR	276.1819	304.1768	FRW	462.2612	490.2561
FRWG	519.2827	547.2776	FRWGK	647.3776	675.3725	RW	315.1928	343.1877
RWG	372.2142	400.2092	RWGK	500.3092	528.3041	RWGKP	597.3620	625.3569
RWGKPV	696.4304		WG	216.1131	244.1081	WGK	344.2081	372.2030
WGKP	441.2609	469.2558	WGKPV	540.3293	568.3242	WGKPVG	597.3507	625.3457
GK	158.1288	186.1237	GKP	255.1816	283.1765	GKPV	354.2500	382.2449
GKPVG	411.2714	439.2663	GKPVGK	539.3664	567.3613	GKPVGKK	667.4614	695.4563
KP	198.1601	226.1550	KPV	297.2285	325.2234	KPVG	354.2500	382.2449
KPVGK	482.3449	510.3398	KPVGKK	610.4399	638.4348	PV	169.1335	197.1285
PVG	226.1550	254.1499	PVGK	354.2500	382.2449	PVGKK	482.3449	510.3398
VG	129.1022	157.0972	VGK	257.1972	285.1921	VGKK	385.2922	413.2871
GKK	286.2238	314.2187	KK	229.2023	257.1972			





NCBI **BLAST** search of SYSMEHFRWGKPVGKKR
(Parameters: blastp, nr protein database, expect=20000, no filter, PAM30)
Other BLAST web gateways

All matches to this query

Score	Mr(calc)	Delta	Sequence
38.4	2092.0789	0.0001	SYSMEHFRWGKPVGKKR
12.1	2092.0701	0.0088	QDNYSLVIFSNQNGIPRK
9.9	2092.0912	-0.0123	ERQAALDSGVLAIAEHEGKV
8.8	2092.0773	0.0016	SIAFDLSSQTSGLNGQRRR
8.5	2092.0841	-0.0052	GQLDVKGLAFQILDAPSSFS
7.4	2092.0912	-0.0123	AARTLQGEEVRSKLTSEFA
7.4	2092.0589	0.0200	SSPGLPQQSFTPQYSLIRS

6.6	2092.0888	-0.0098	CFYVQVEQRKQPELRGL
6.6	2092.0675	0.0115	RDQQRSQALVDLHRSFH
6.6	2092.0589	0.0200	DFFKVSASEAAAIDPQQRL

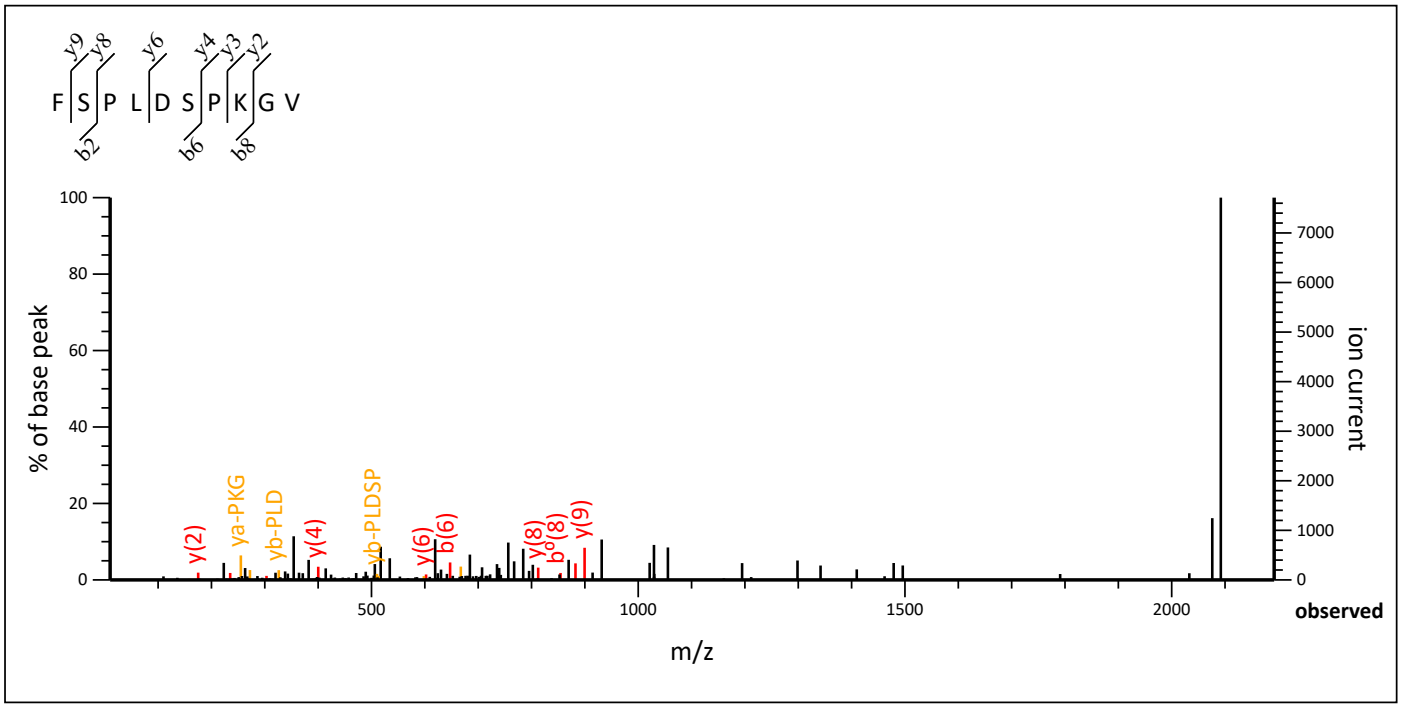
Mascot: http://www.matrixscience.com/

Mascot Search Results

Peptide View

MS/MS Fragmentation of **FSPLDSPKGV**
Found in **DAPB_ASPCL** in **SwissProt**, Probable dipeptidyl-aminopeptidase B OS=Aspergillus clavatus (strain ATCC 1007 / CBS 513.65 / DSM 816 / NCTC 3887 / NRRL 1) OX=344612 GN=dapB PE=3 SV=1

Match to Query 1: 1045.534524 from(1046.541800,1+) intensity(1.0000) index(0)
Title: Reading Top-Down experiment
Data file 1047.txt



10.07 to 2192.1

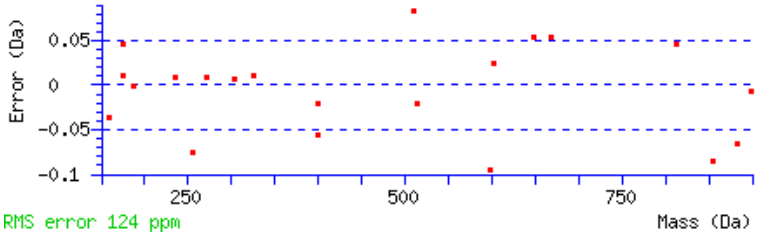
Label all possible matches ○ Label matches used for scoring ◉

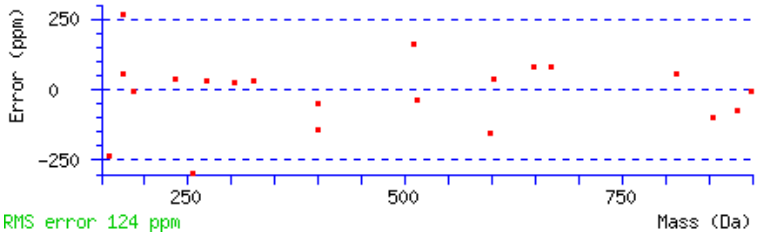
Monoisotopic mass of neutral peptide Mr(calc): 1045.5444
Ions Score: 21 **Expect:** 54
Matches : 21/103 fragment ions using 54 most intense peaks (help)

#	Immon.	b	b*	b^0	Seq.	y	y*	y^0	#
1	120.0808	148.0757			F				10
2	60.0444	**235.1077**		217.0972	S	***899.4833***	882.4567	881.4727	9
3	70.0651	332.1605		314.1499	P	***812.4512***	795.4247	794.4407	8
4	86.0964	445.2445		427.2340	L	715.3985	698.3719	697.3879	7
5	88.0393	560.2715		542.2609	D	***602.3144***	585.2879	584.3039	6
6	60.0444	**647.3035**		629.2930	S	487.2875	470.2609	469.2769	5
7	70.0651	744.3563		726.3457	P	***400.2554***	383.2289		4
8	101.1073	872.4512	855.4247	854.4407	K	***303.2027***	286.1761		3
9	30.0338	929.4727	912.4462	911.4621	G	***175.1077***			2
10	72.0808				V	118.0863			1

Seq	ya	yb	Seq	ya	yb	Seq	ya	yb
SP	157.0972	185.0921	SPL	270.1812	298.1761	SPLD	385.2082	413.2031
SPLDS	472.2402	500.2351	SPLDSP	569.2930	597.2879	SPLDSPK	697.3879	

PL	183.1492	211.1441	**PLD**	298.1761	326.1710	**PLDS**	385.2082	413.2031
PLDSP	482.2609	510.2558	**PLDSPK**	610.3559	638.3508	**PLDSPKG**	667.3774	695.3723
LD	201.1234	229.1183	**LDS**	288.1554	316.1503	**LDSP**	385.2082	413.2031
LDSPK	513.3031	541.2980	**LDSPKG**	570.3246	598.3195	**DS**	175.0713	203.0662
DSP	272.1241	300.1190	**DSPK**	400.2191	428.2140	**DSPKG**	457.2405	485.2354
SPK	285.1921	313.1870	**SPKG**	342.2136	370.2085	**PK**	198.1601	226.1550
PKG	255.1816	283.1765	**KG**	158.1288	186.1237			





NCBI **BLAST** search of FSPLDSPKGV
(Parameters: blastp, nr protein database, expect=20000, no filter, PAM30)
Other BLAST web gateways

All matches to this query

Score	Mr(calc)	Delta	Sequence
20.6	1045.5444	-0.0099	FSPLDSPKGV
14.0	1045.5345	0.0000	DRVYIHPF
13.1	1045.5280	0.0065	KHLMHHFP
12.2	1045.5291	0.0054	DAIKLVDSGE
11.6	1045.5404	-0.0059	GQLTGKKADE
11.6	1045.5444	-0.0099	YVSSPLPQGV
11.5	1045.5305	0.0040	DDRFIQPR
11.4	1045.5444	-0.0099	FDSLLANPVA
11.2	1045.5291	0.0054	NATLLLGTDE
10.6	1045.5444	-0.0099	DNGLLSALPF

Mascot: http://www.matrixscience.com/